Strain Induced Surface Reconstructions of Compound Semiconductor Alloys

by **N. A. Modine, J. E. Bickel*, A. Van Der Ven*, C. A. Pearson**, and J. Mirecki Millunchick***

Motivation—The nanoscale structure of crystalline surfaces is controlled by competing interactions between the constituent atoms. For example, compound semiconductor surfaces typically reconstruct in order to eliminate dangling bonds and reduce their surface energy. It is generally accepted that three principal factors influence the stable surface reconstruction: local chemistry, the electron counting rule, and local strain due to the displacement of atoms from their bulk positions. These factors readily explain the surface reconstructions present in binary III-V semiconductor systems. However, when alloying occurs, coexistence of nanoscale domains of multiple reconstructions and new reconstructions not observed for the binary systems suggest that other factors also contribute. We propose that global lattice mismatch strain and localized atomic size mismatch strain are additional factors that greatly influence the surface structure of compound semiconductor alloys.

Accomplishment—InAs and GaAs both form stable surfaces of a single reconstructions varying from c(4x4) to β2(2x4) to α2(2x4) to (4x2) as a function of chemical potential μ. The ternary alloy InGaAs, however, shows multiple reconstructions for a single μ. For example, on $In_{0.27}Ga_{0.73}As$/GaAs, a (4x3) reconstruction unique to the alloy system coexists with nanoscale domains of what appears to be an α2(2x4) reconstruction. Studies of the α2(2x4) show that the surface dimer, rather than being stochastically distributed between the two possible positions instead regularly alternates position 80% of the time. *Ab Initio* studies based on the Kohn-Sham Density Functional Theory show that localized strain due to ordering of indium atoms in the first subsurface layer induces an ordering of the surface dimers. These results demonstrate the important influence of atomic size mismatch strain on the surface reconstructions of alloyed compound semiconductor systems.

A coexistence of surface reconstructions also occurs when thin films of GaSb are grown on GaAs. The film develops by nucleating small islands of α(4x3). The center of these islands transform to the α2(2x4) reconstruction above the critical island size of $30\pm10 nm^2$. The lattice mismatch of film and surface is 7%, and DFT simulations suggest this drives the surface coexistence. The α(4x3) is stable at the GaSb lattice parameter, whereas the α2(2x4) is stabilized at the GaAs lattice parameter. At the center of the island where the lattice parameter is constrained to that of the substrate, the α2(2x4) appears, whereas at the edge of the island where the lattice parameter can elastically relax, an α(4x3) reconstruction appears. This demonstrates the important influence of lattice mismatch strain on the surface reconstructions of alloyed compound semiconductor systems.

Significance—Surface reconstructions play an important role in the growth of thin films and devices, influencing the compositional and morphological structure of the grown material at the nanoscale. It is important to understand the surface structure in order to control the nanoscale structure of devices made of III-V semiconductors.

*** University of Michigan, Ann Arbor**
**** University of Michigan, Flint**

Sponsors for various phases of this work include: DOE Office of Basic Energy Sciences/Center for Integrated Nanotechnologies (CINT)
Contact: Normand A. Modine, CINT Science, Dept. 1132
Phone: (505) 844-8412, Fax: (505) 284-7778, E-mail: namodin@sandia.gov

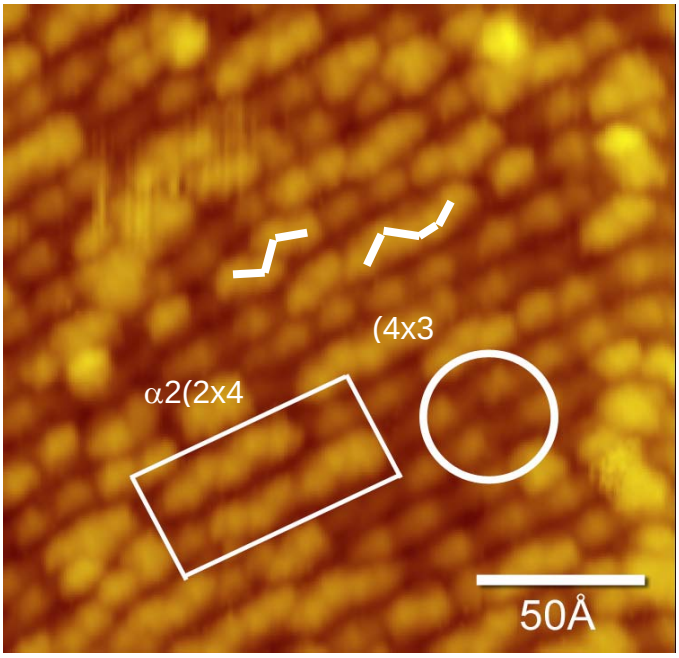

Figure 1. Scanning Tunneling Microscope (STM) image of a 25 monolayer film of $In_{0.27}Ga_{0.73}As$ grown on GaAs at 493°C. Nanoscale domains of α2(2x4) exist within a matrix of a (4x3) unique to the alloy system, and the alternation of the α2(2x4) surface dimer is apparent.

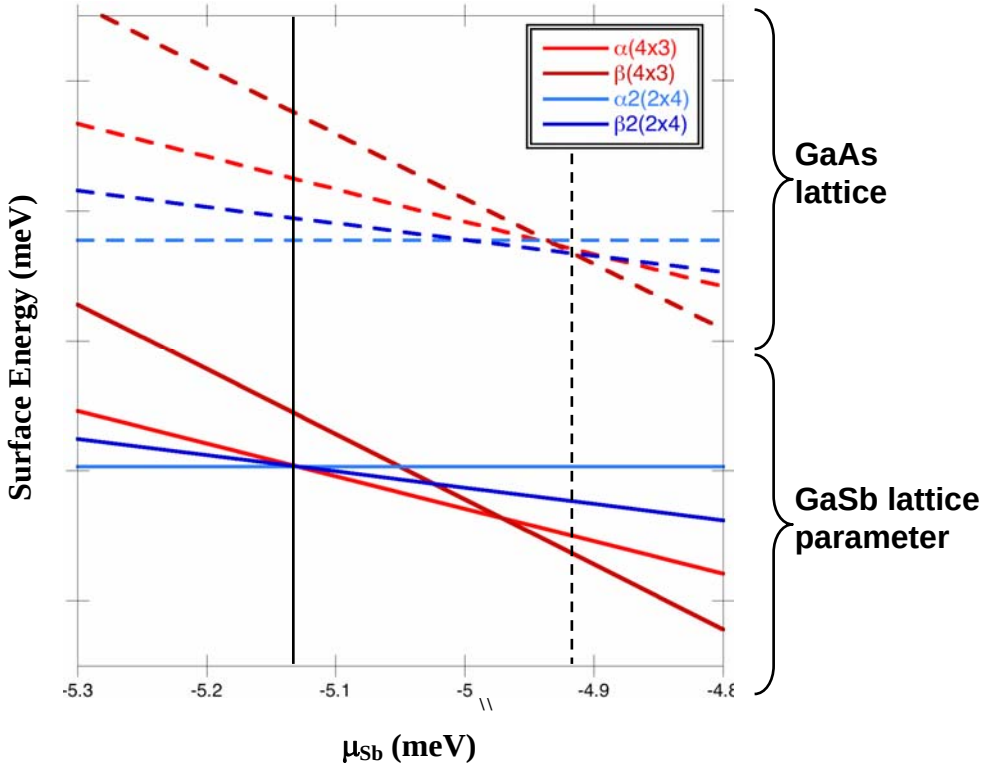

Figure 2. Surface energies of various reconstructions of GaSb calculated with the Density Functional Theory (DFT) as a function of chemical potential. Under growth conditions, the (4x3) is stable at the GaSb lattice parameter, while the (2x4) is stable at the GaAs lattice parameter.